

Table S7 .Structural and energetic parameters for the cyclic sulfenyl amide formation in water

Parameter	Peptide in water		
ΔE	-1.5 kcal/mol		
Eact	9 kcal/mol		
	Reactive	TS	Product
N-CA-C-N+1	-155	-154	-109
dSO	1.73	2.23	2.4
dNH	1.03	1.58	2.63
dSN	2.81	1.92	1.83
dH _{NH} O _w	1.83	1.06	1.02
qS	0.012	0.018	-0.16
qOH	-0.158	-0.032	-0.028
qH _{NH}	-0.16	-0.044	0.002
qN	0.354	0.126	0.156